Using Rapid Analytical Results for On-site Decision Making During Site Inspections

Deana M. Crumbling, M.S.
Technology Innovation Office
U.S. Environmental Protection Agency
Washington, D.C.
(703) 603-0643
crumbling.deana@epa.gov

May 8 & 9, 2003
EPA National Site Assessment Conference, Pittsburgh

USEPA
Technology Innovation Office

- Advocates for better technologies and strategies to clean up contaminated sites:
  - Site investigation/characterization
  - Site remediation
  - Monitoring during or after remedial action
- Acts as an agent for change
  - Disseminates others' good ideas
- Cleanup Information Website: http://cluin.org

Take-Home Message

Why is it important to use new sampling and analytical technologies?

Because generating good quality data takes MORE than "perfect" chemical analysis!

It requires that samples be "representative."

For environmental matrices, just what does "good" data quality and "representative data" mean?

The Concept of "Representative Data" Should be Intricately Linked to an Accurate Conceptual Site Model

Correct Decisions are Based on an Accurate CSM

- Correct decisions about sites require an accurate (i.e., representative of reality) Conceptual Site Model (CSM)

- A CSM is any depiction (graphical or verbal) of what contamination exists (or might exist); how it (might have) got(ten) there; where it is (might be) located; where it might be migrating to or what it might degrade into; who might be exposed (harmed) through intact exposure pathways. This information is inseparable from what might be done to prevent that exposure/harm.

Conceptual Site Model

A CSM is any tool(s) that lets you represent, "conceptualize" or "model" site contamination issues and concentration populations so you can make predictions about nature, extent, risk, and risk reduction strategies

For confident project decision-making to occur, relevant uncertainties in the CSM must be managed so that intolerable decision errors are avoided.

Data is usually used to decrease CSM uncertainty.

Conceptual Site Model Considerations

- **How** the contaminant release occurred will dictate where the contamination might be located, as well as how heterogeneous (patterned) contaminant distributions are.
- **What** are contaminant dispersal mechanisms or likely fate of the contaminants? Would these be expected to augment or reduce heterogeneity?
- **Who** might be exposed to the contaminants or degradation products in the present or the future?
- If so, what are likely or possible risk reduction mechanisms that would be consistent with project constraints?
- An accurate, mature CSM will delineate contaminant populations for which the decisions or outcomes will differ.

Achieving Project Decision Quality

- Correct project decisions (decision quality) are dependent on an accurate CSM
- What constitutes an inaccurate CSM?
  - Estimates of contaminant presence and location differ enough from "true" to such a degree that decisions are different from what would have been made if "true" were known.
- When is an inaccurate CSM unacceptable?
  - When the consequences of the resulting decision errors produce "intolerable" consequences (e.g., potential for excessive exposures, excessive costs, or avoidable failure of a remedial design)

Predicted GW CSMs Based on Traditional Well Sampling vs. High Density Sampling

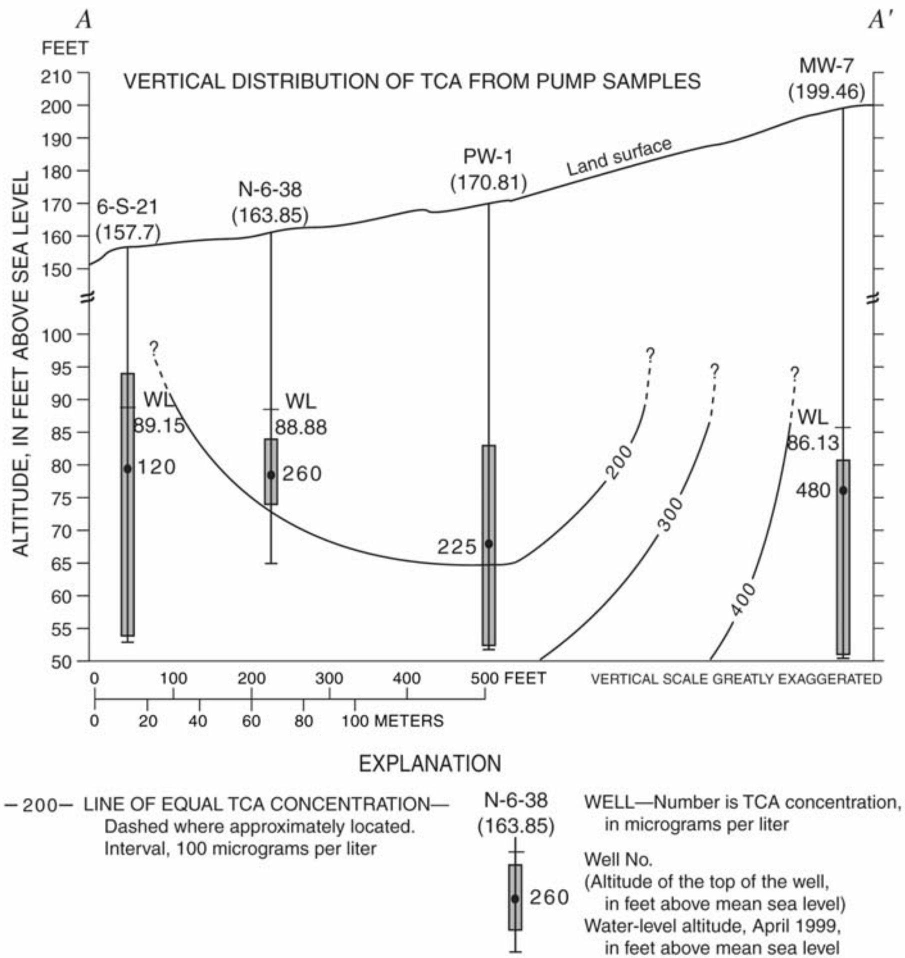


Figure 6. Vertical distribution of TCA concentrations in ground-water samples collected with the diffusion samplers and submersible pump.

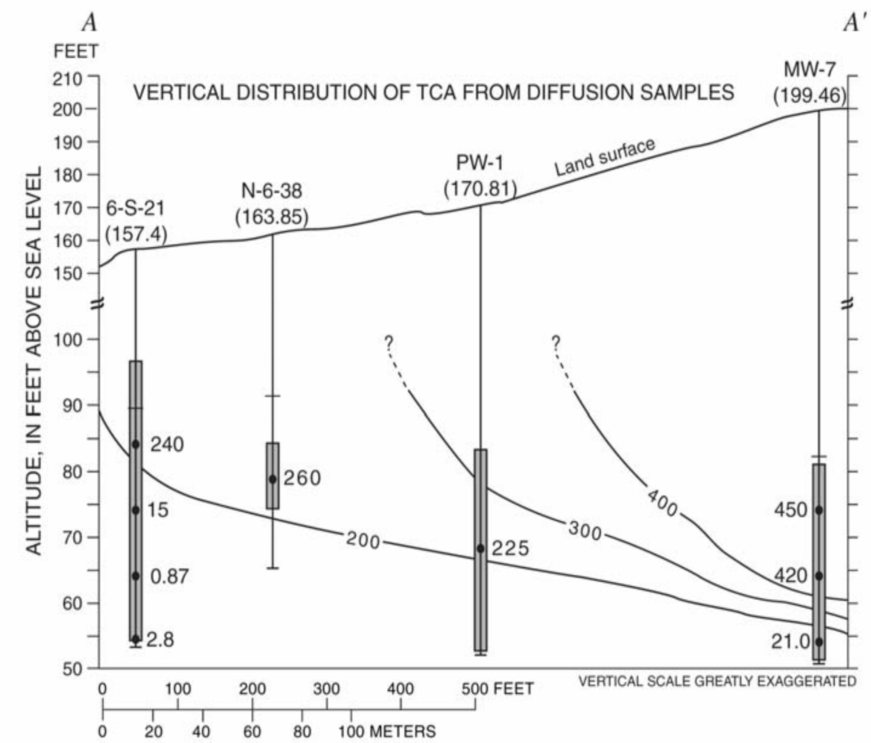


Figure 6.—*Continued.*

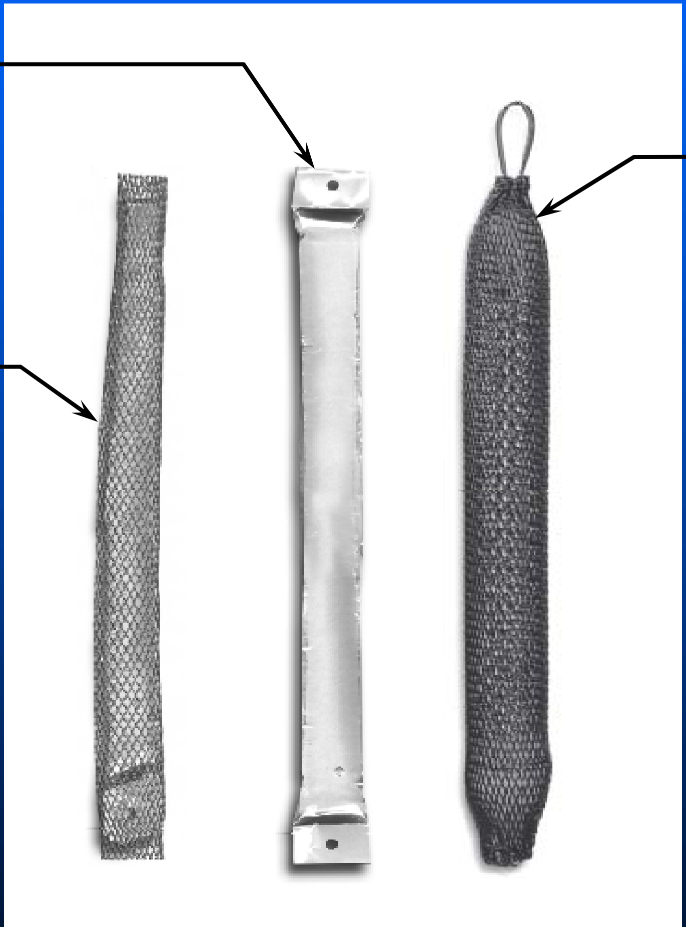
From USGS Report 02-4203 (2002)

Typical Water-Filled PDB Samplers

PDB sampler without protective mesh

PDB sampler attached to bailer bottom

PDB sampler with protective mesh

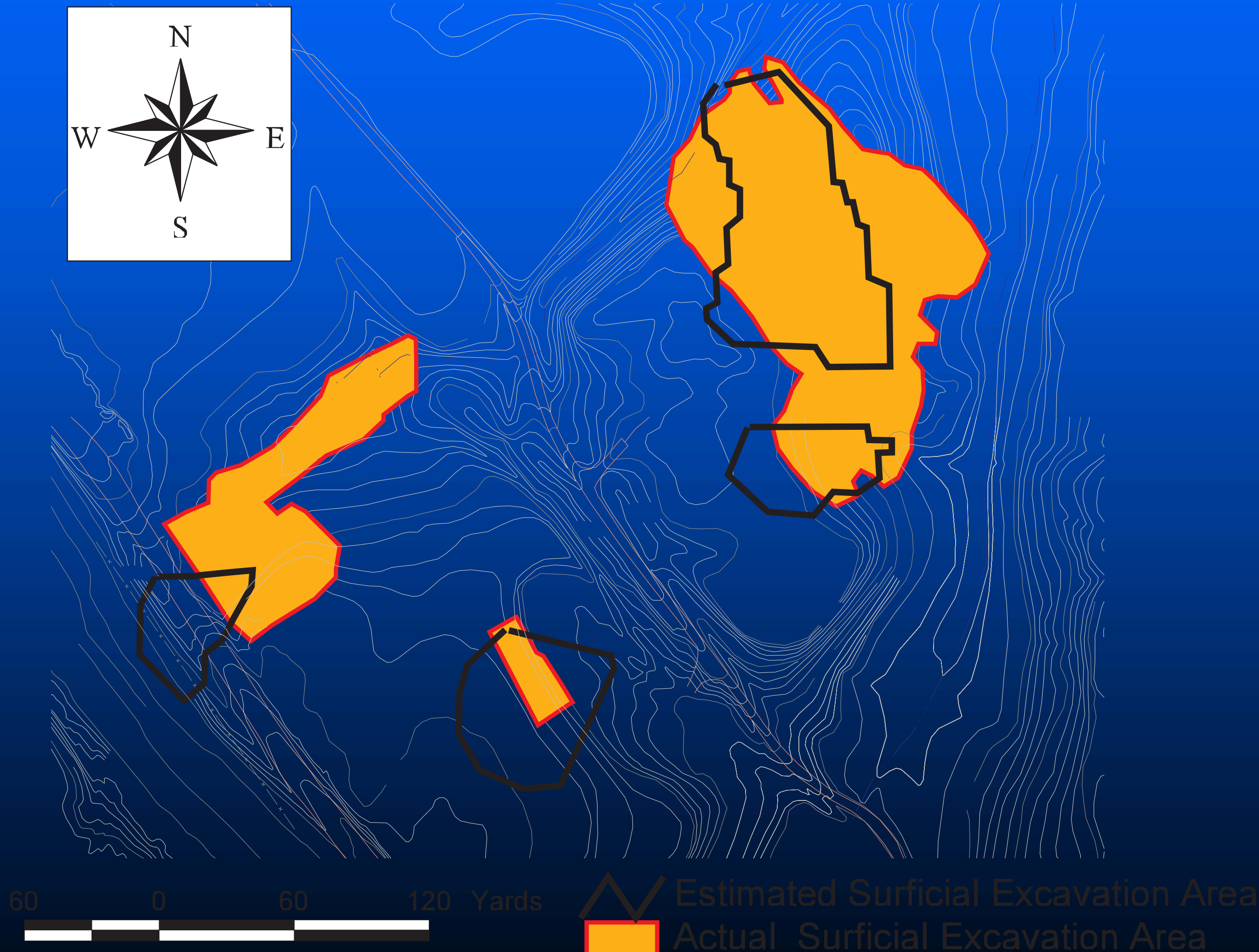


Must purchase from vendor or obtain license from USGS (703 648:4344)

For more info, see archived Internet seminar/PPT file on Clu-In Website below

Slide adapted from http://www.clu-in.org/conf/itrc/diffusion_032602/

Cleanup Design CSM Projected from RI Data (black) vs. Actual Contamination Boundaries Developed by Focused, High Density Sampling (orange)



If data leads to the wrong conclusions, would you call it "good quality data"?

Adapted from Argonne, 2002

Most data uncertainty
(and thus uncertainty in the accuracy of the CSM)
stems from uncertainty about "data representativeness"

Why?

Because usually there are not enough samples to characterize a heterogeneous matrix well enough to produce an accurate CSM at scales relevant to risk and remedy decisions

Emerging tools cost-effectively increase sampling density to support accurate CSMs

Passive Diffusion Samplers Have Small Sample Supports that Detect Vertical Conc. Gradients…

From USGS Report 02-4203 (2002)

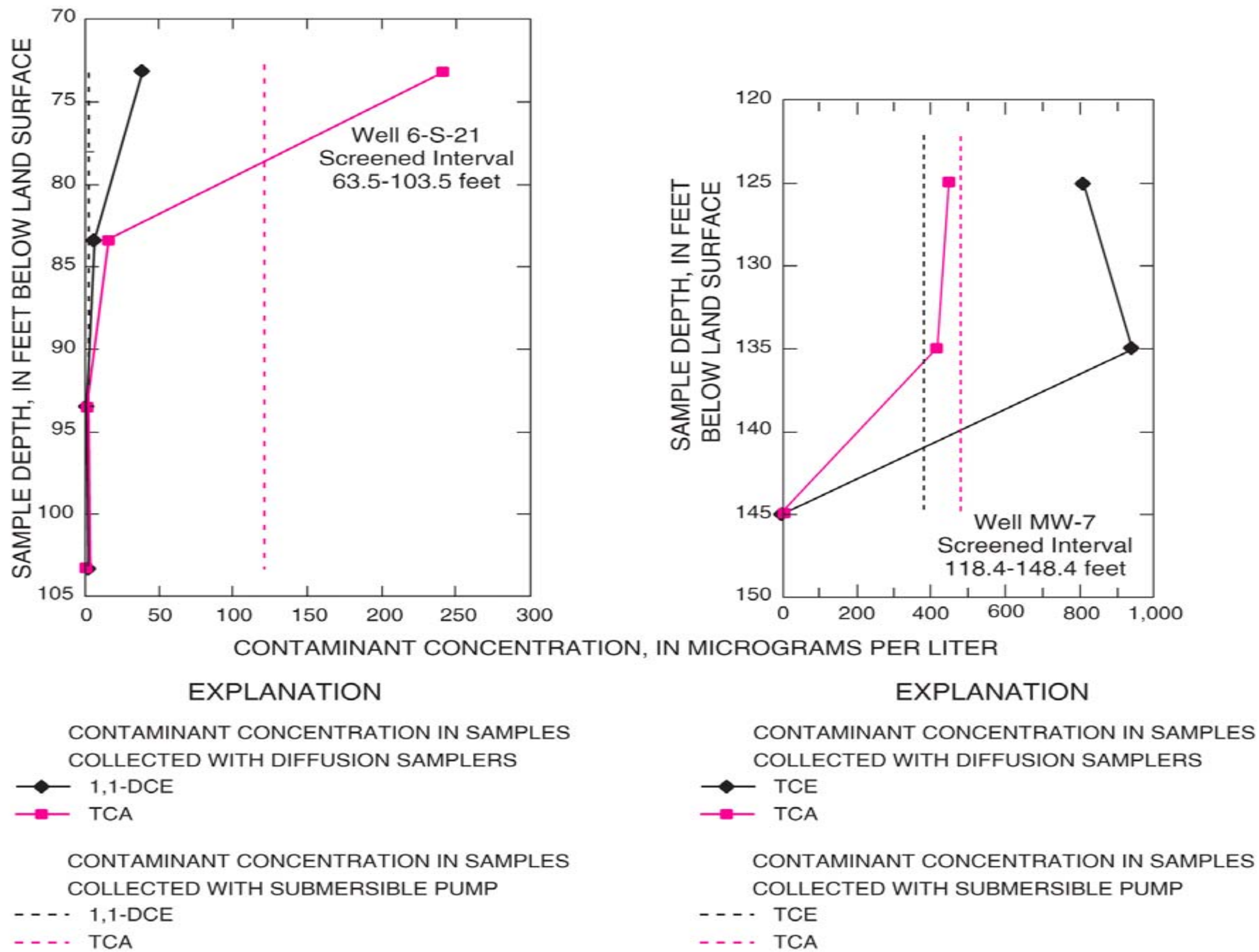


Figure 5. Comparison of selected volatile organic compound concentrations from ground-water samples collected with diffusion samplers and a submersible pump for wells with greater than 20-foot screened intervals in Area 6, Naval Air Station Whidbey Island, Washington.

…Avoiding the Uncontrolled Mixing of Distinct Populations that Produces Inaccurate CSMs

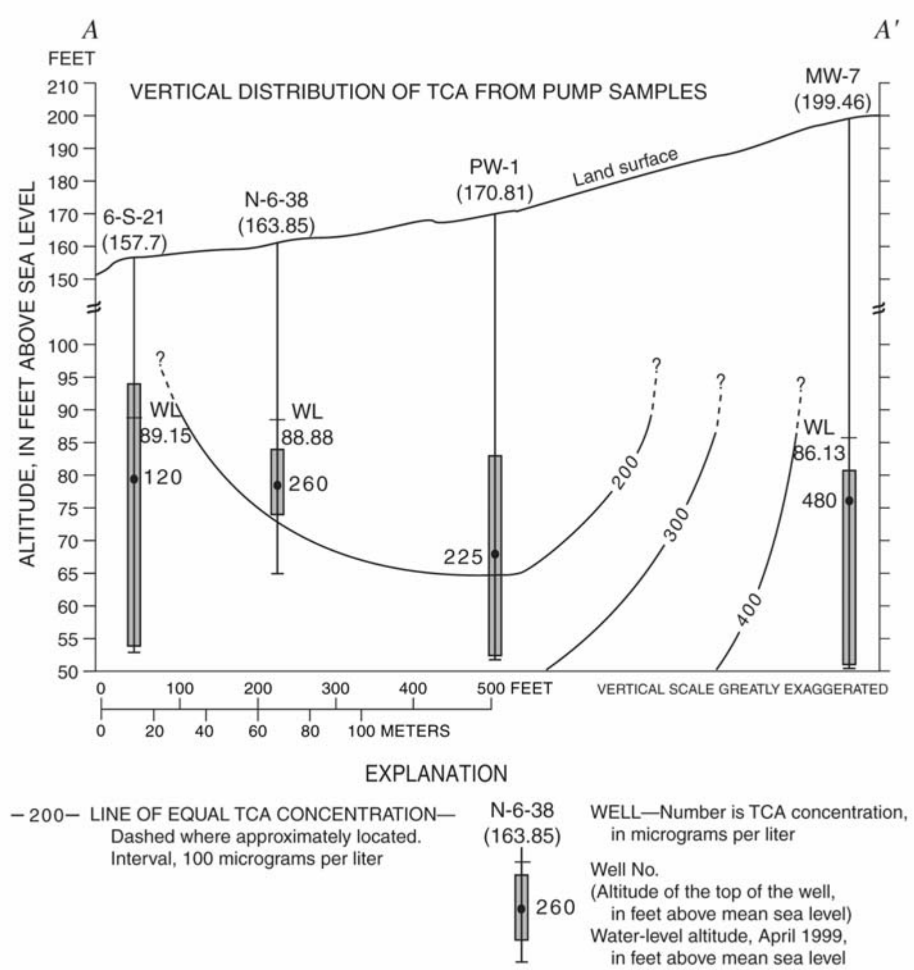


Figure 6. Vertical distribution of TCA concentrations in ground-water samples collected with the diffusion samplers and submersible pump.

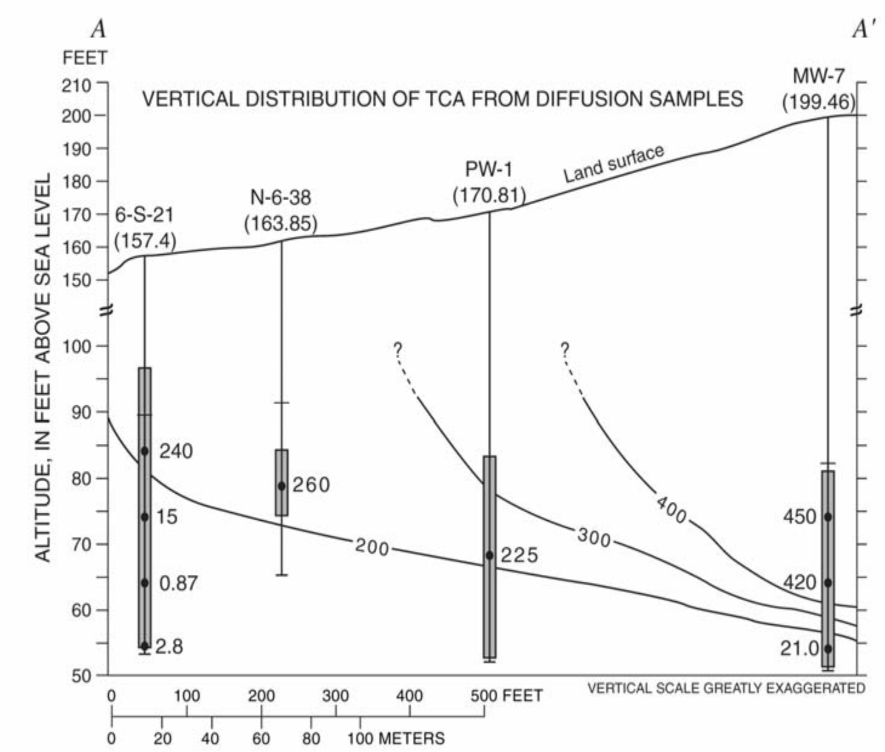
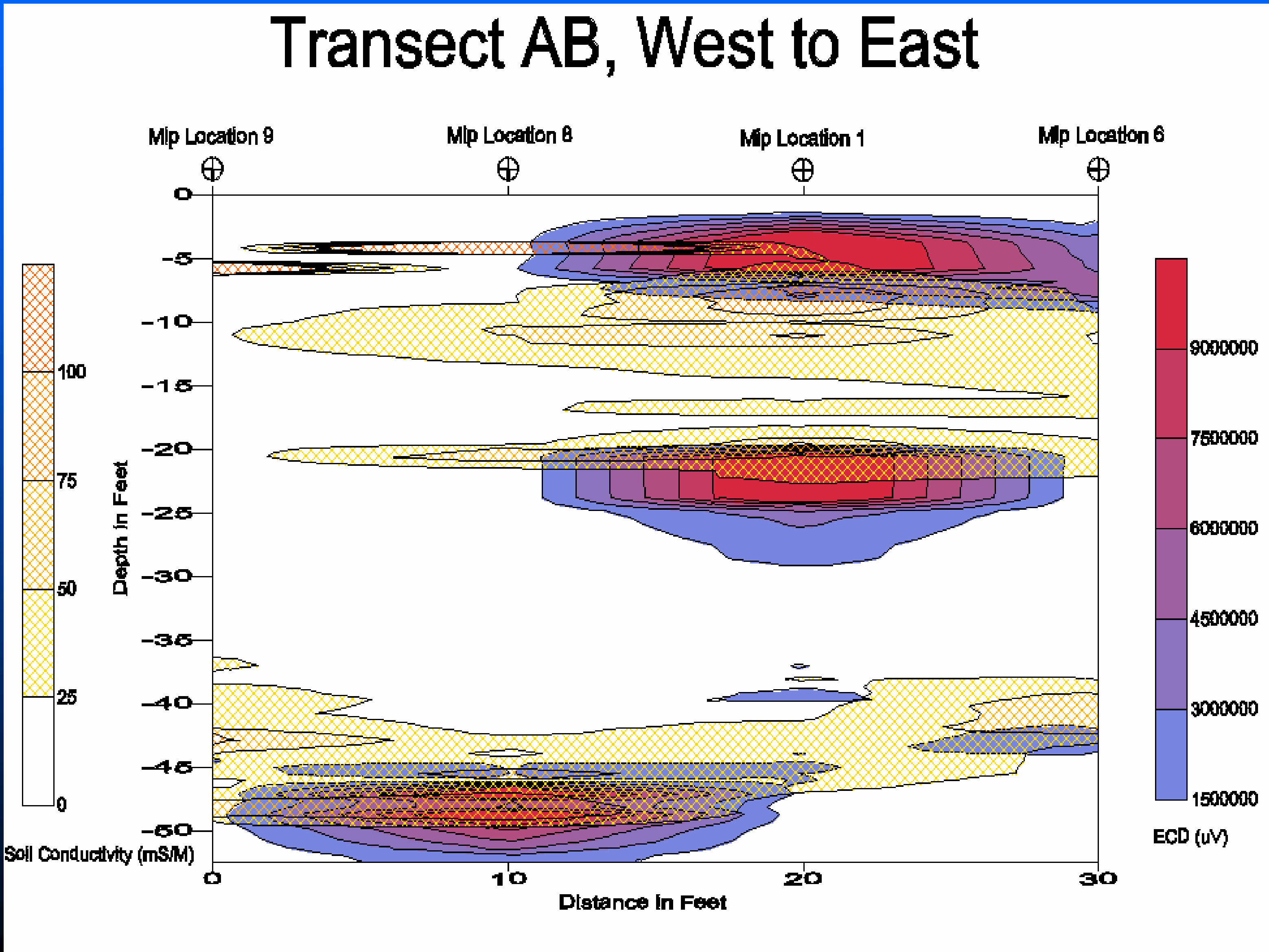


Figure 6.—*Continued.*

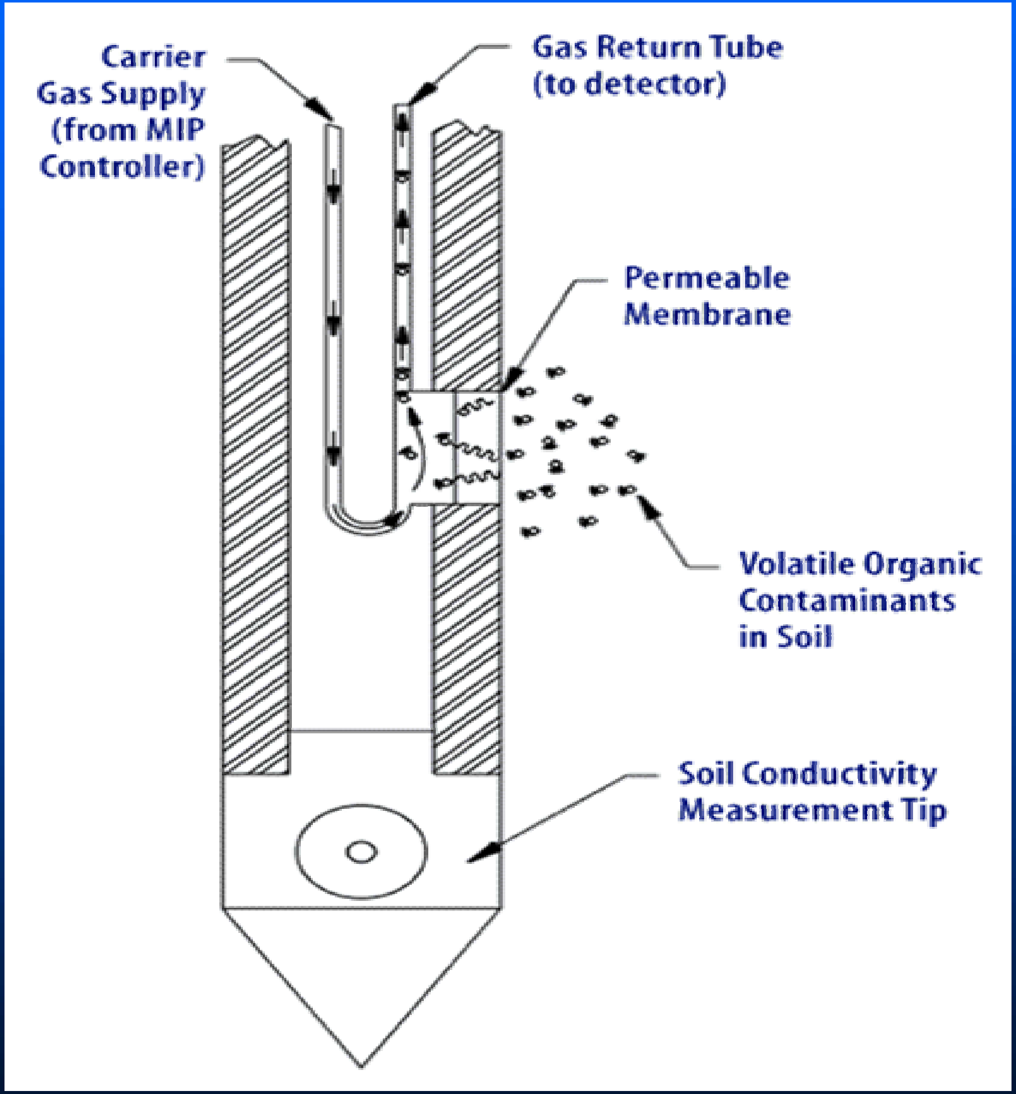
From USGS Report 02-4203 (2002)

Direct Push-Membrane Interface Probe (DP-MIP) provides a smaller (*in situ*, real-time) sample support that gives a truer representation of heterogeneous GW contamination



Graphic courtesy of Columbia Technologies, Inc.

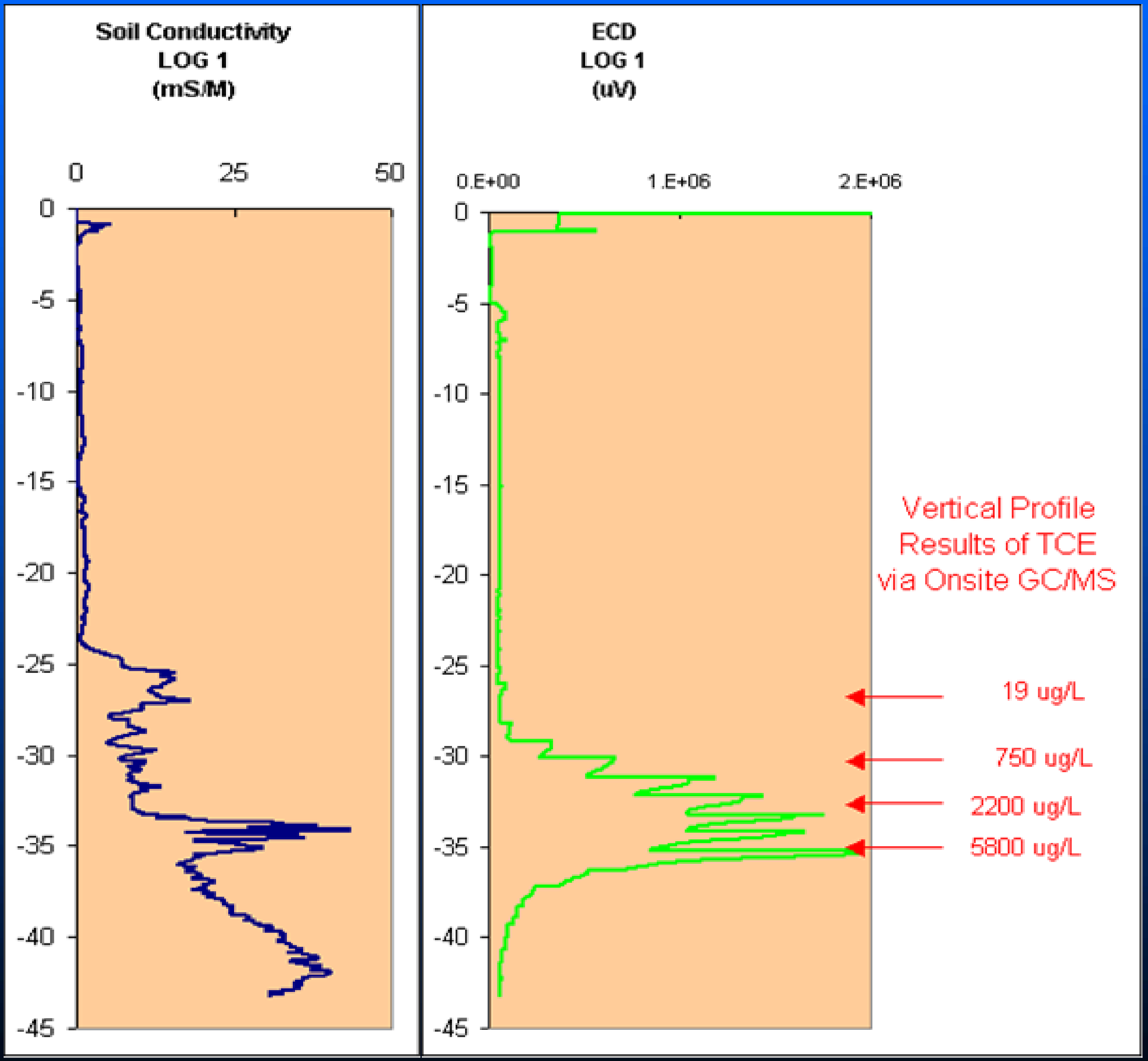
MIP Principles of Operation



- Heated probe
- Semi-permeable membrane
- Contaminant vapors partition into a carrier gas
- Transported to FID, PID, & ECD detectors at the surface
- Results are displayed in real-time on a lap-top computer.
- For more info, go to http://fate.clu-in.org/direct_push/dpanalytical.asp

Slide adapted from Columbia Technologies, Inc., 2001

A DP-MIP can take measurements every 2 inches as it is pushed



MIP = membrane-interface probe (w/ ECD detector)

Graphic courtesy of Columbia Technologies, Inc.

Updating the Environmental Data Quality Model to Accept New Tools that Manage Data Uncertainty

Oversimplified (First-Generation) Data Quality Model

Methods = Data = Decisions

Screening Methods	→	Screening Data	→	Uncertain Decisions
"Definitive" Methods	→	"Definitive" Data	→	Certain Decisions

This Model Fails to Distinguish:
Analytical Methods from Data from Decisions

Inaccurate First Generation Assumptions

- "Data quality" depends on analytical methods
- Using regulator-approved methods ensures "definitive data"
- Contaminant concentrations and behaviors are nearly uniform across scales of environmental decision-making
- Impacts of spatial variability can be ignored & results from tiny samples can be extrapolated to represent large matrix volumes
- QC checks that use ideal matrices are representative of method performance for real-world samples
- Laboratory QA is substitutable for project QA
- One-size-fits-all methods eliminate the need for analytical chemistry expertise

So, What is "Good Quality" Data?

- Quality = "the totality of *features* and *characteristics* of a product or service that bear on its ability to meet the stated or implied needs and expectations of the user" (USEPA OEI QMP 2000, v. 1.3) = "fitness for use."
- Quality assurance (QA) activities seek to avoid mistakes that degrade the fitness of a product or service.
- The bottom line for site cleanup regulatory programs is to ensure that decisions about sites' risks, risk reduction strategies, and reuse are correct…so that decisions made by regulators and RPs can be trusted (i.e., decisions are fit for use).

The Foundation of a Better Data Quality Model

Data Quality = Should be assessed according to the ability of data to provide information that meets user needs

- Users need to make correct decisions
- Therefore, data quality is a function of data's…
  - Ability to represent the "true state" (of the decision unit) in the context of the decision the data user wants to make
  - In other words, data's ability to support a CSM that accurately represents the site at a scale commensurate with the scale of decision-making

Data Quality: More than Just Analysis

Perfect Analytical Chemistry + **Non-Representative Sample(s)**

"BAD" DATA

Distinguish:
Analytical Quality from Data Quality

The concept of "representativeness" must be grounded in the decision context

Different decisions require different representativeness.

For example:

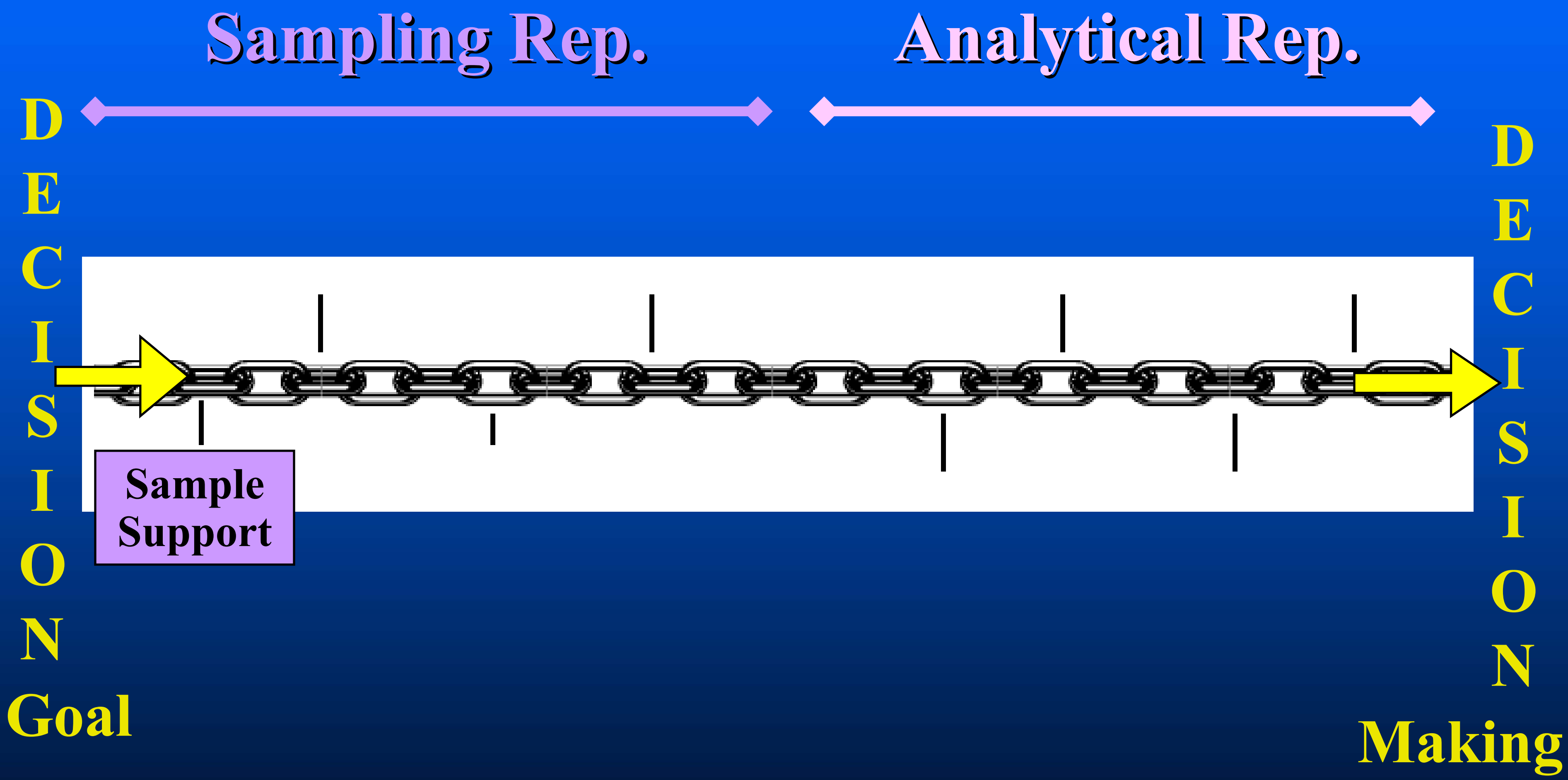
- A data set <u>representative of</u> a risk assessment decision usually needs to estimate the average concentration over a fairly large decision unit (called an "exposure unit")
- A data set <u>representative of</u> a cost-effective remedial design must provide information about concentration extremes and distributions at a scale specific to the remedial option considered.
- Scales for treatment technologies vary with the technology (e.g., the scale of characterization for successful chemical oxidation is much finer than for deploying *in situ* heating).
- Institutional control scales usu. larger than scales for treatment.

Generic Sampling Designs Cannot be Expected to Produce Representative Data for Heterogeneous Matrices

It is impossible to specify a one-size-fits-all data set that could be representative of all potential site decisions!

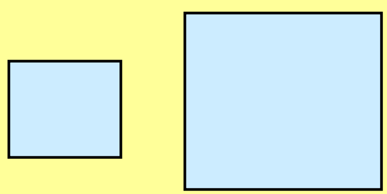
Therefore, the first step of ensuring data quality is to clearly understand to what decisions the data will be applied.

The Data Quality "Chain"



Sample Support: Size Matters!

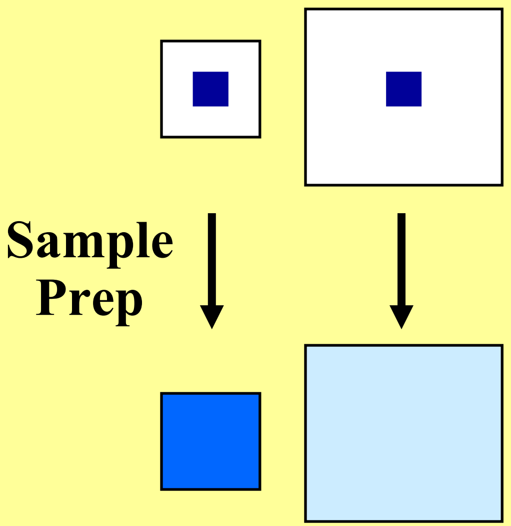
Typical regulatory and field practices assume that the size/volume of a sample has no effect on analytical results for contaminant concentrations.



That assumption doesn't hold true when environmental heterogeneity exists;

sample volume can determine the analytical result!

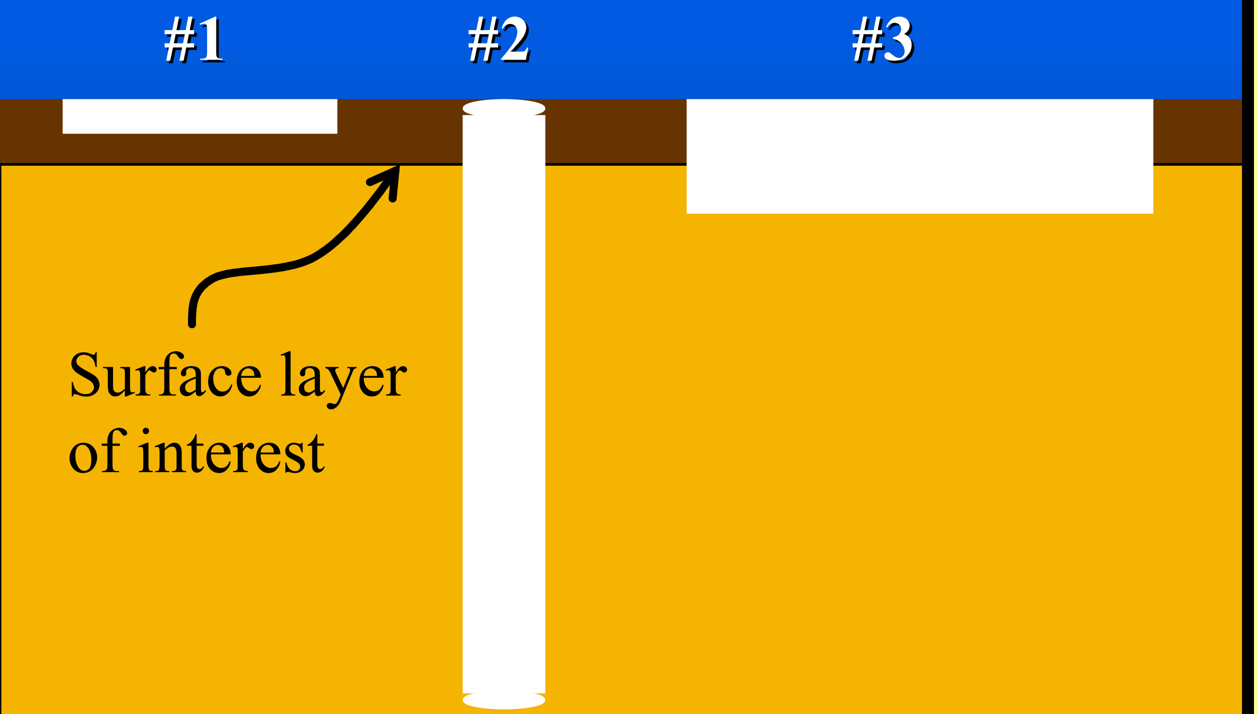
The Nugget Effect



Although there is the same contaminant mass in the captured nuggets, different volumes of cleaner matrix will produce different sample concentrations after sample homogenization.

Sample Support: Critical to Representativeness

"Sample support" includes spatial orientation

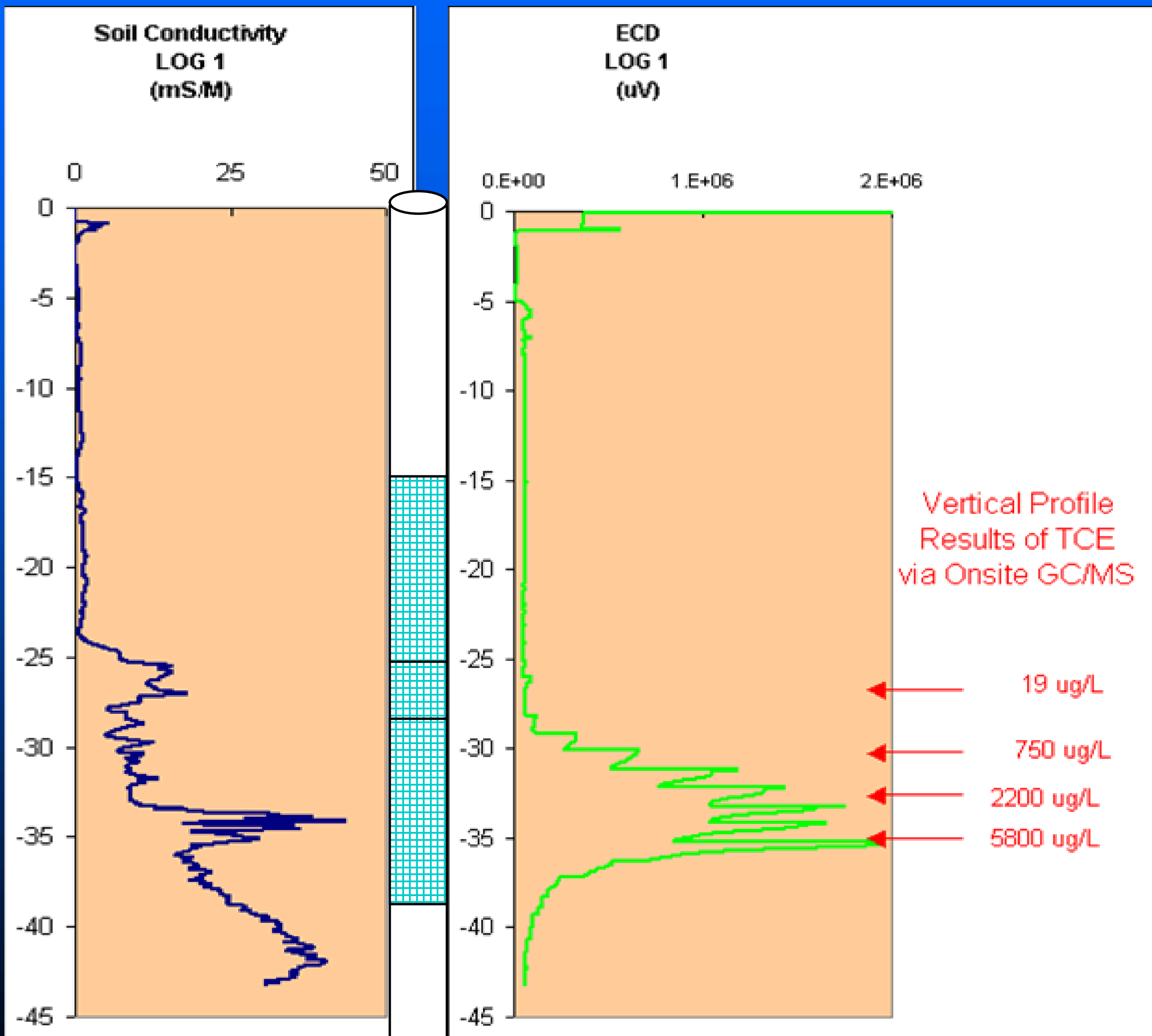


The decision driving sample collection:
Assess contamination resulting from atmospheric deposition

Given that the dark surface layer is the soil layer impacted by atmospheric deposition relevant to this project:

Which sample support (white areas #1, #2, or #3, each homogenized before analysis) provides a sample that is representative of atmospheric deposition for this site?

Comparison of MIP to Discrete Sampling w/ GC/MS Results



MIP = membrane-interface probe (w/ ECD detector)

Sample support for MIP on mm-scale

Sample support for discrete field GC/MS on inch-scale

Cf to sample support for traditional well = 10’s of feet

Graphic courtesy of Columbia Technologies

Sample Supports for Passive Diffusion Samplers Are Governed by the Degree of Vertical Mixing

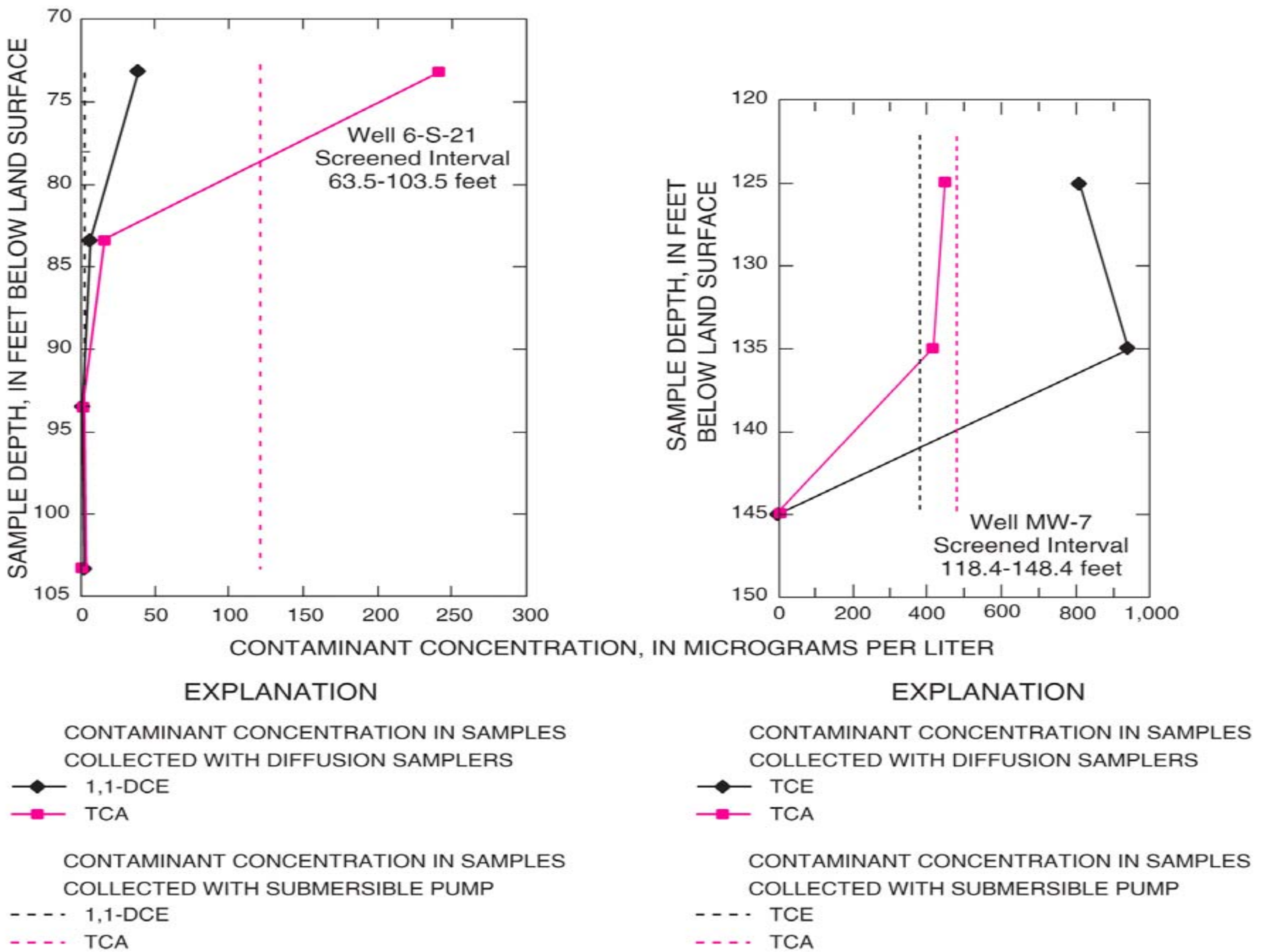


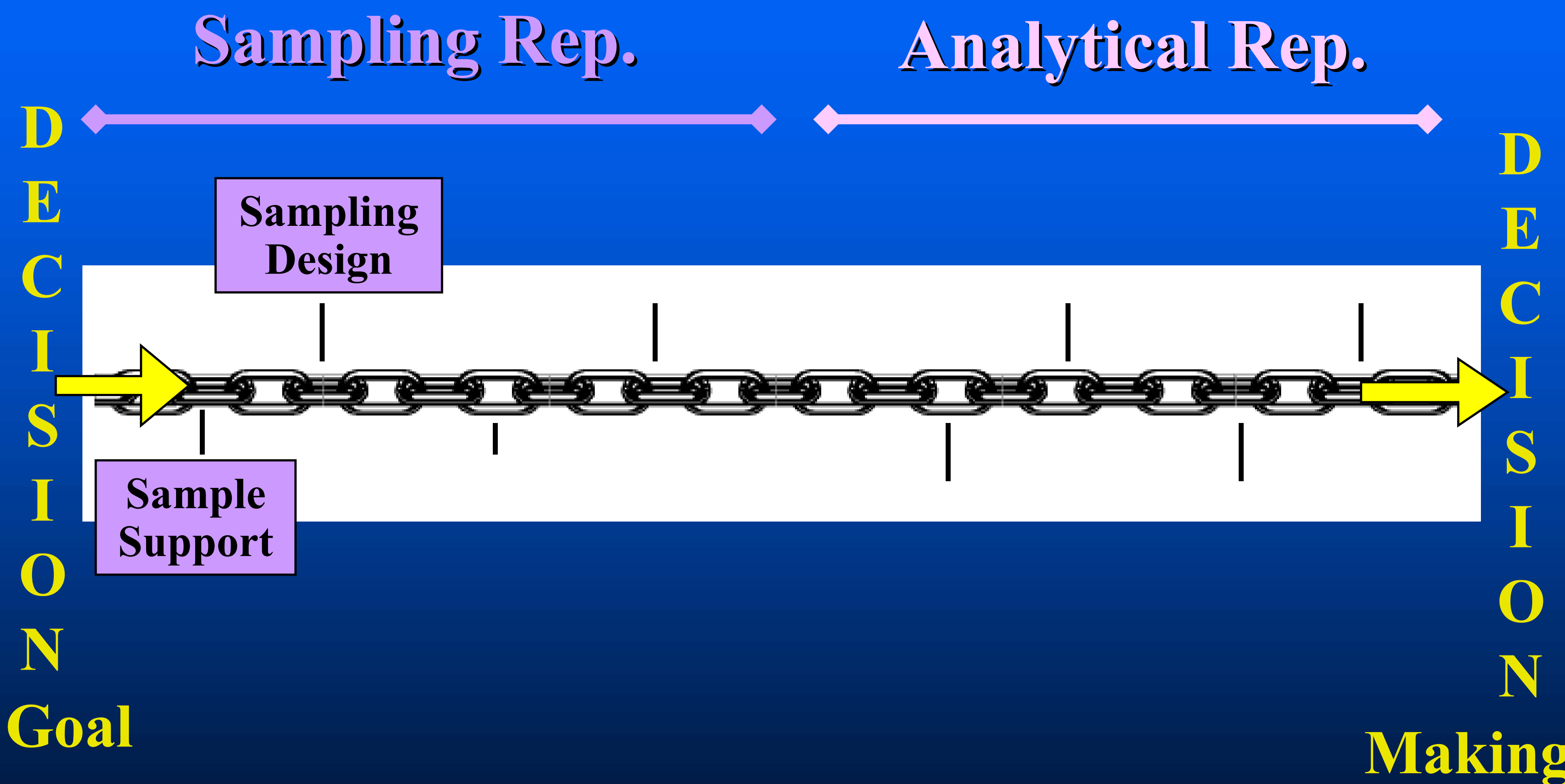
Figure 5. Comparison of selected volatile organic compound concentrations from ground-water samples collected with diffusion samplers and a submersible pump for wells with greater than 20-foot screened intervals in Area 6, Naval Air Station Whidbey Island, Washington.

From USGS Report 02-4203 (2002)

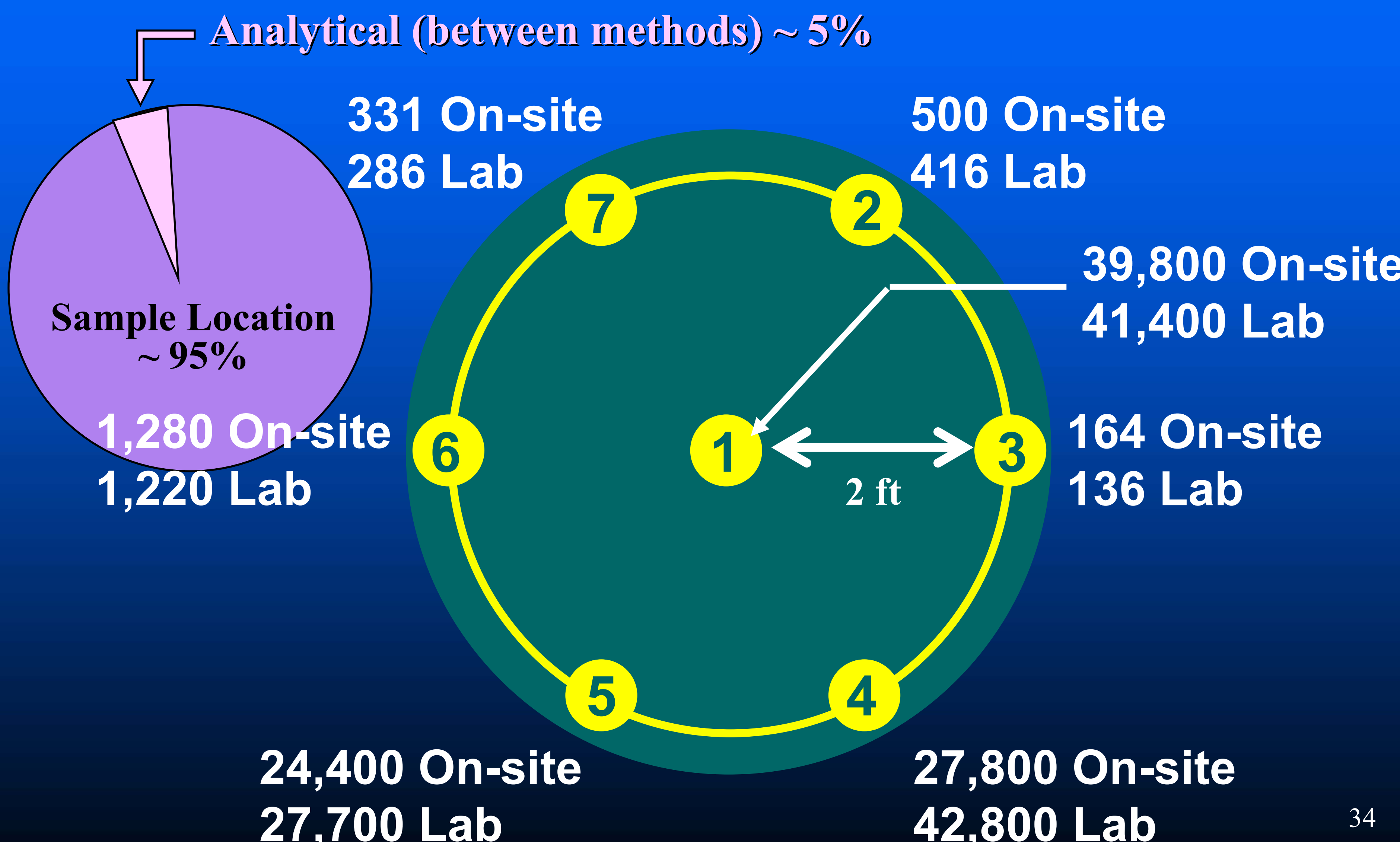
Decision Support guides Sample Support

- How do you decide what sample support is correct?
- The sample support needs to be representative of the "decision support"
- Decision support = the physical properties or characteristics of the decision unit. Includes things like:
  - Matrix volume and dimensions (Ex: air deposition layer)
  - Particle sizes that are of exposure concern (Ex: fine particles with high lead concentrations that facilitate hand-mouth transmission or can be tracked or wind-blown into residences)
  - Should monitoring well data be representative of DW for exposure assessment (implies large sample support)? Or should it be representative of aquifer properties that control contaminant fate & migration or treatment success (implies small sample support)?
- If decision specifics unknown, then decision support unknown, and it is *impossible to plan for representative data collection*!!!

The Data Quality "Chain"



Can Your Sampling Design Detect the Impact of Spatial Heterogeneity?

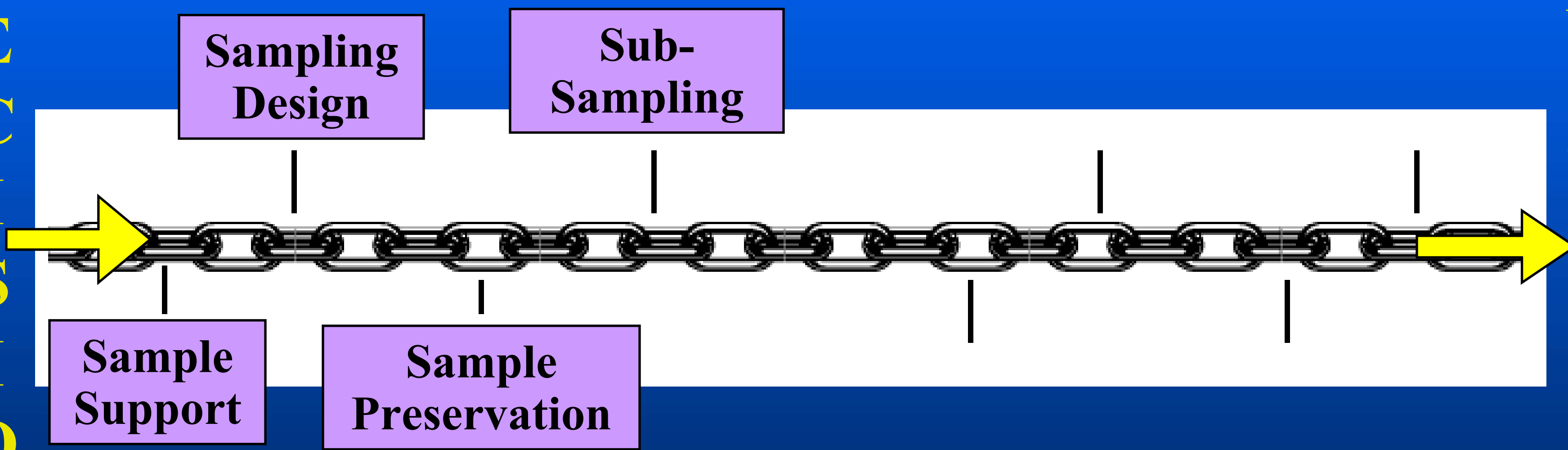


The Data Quality "Chain"

Sampling Rep.

Analytical Rep.

DECISION Goal



DECISION Making

e.g., Method 8270 = GC-MS for SVOCs

All links in the Data Quality chain must be intact for data to be representative of the decision!

Is the Subsample Support Representative?
Lead Concentration Varies w/ Particle Size

Soil Grain Size (Standard Sieve Mesh Size)	Soil Fraction-ization (%)	Pb Conc. in fraction by AA (mg/kg)	Lead Distribution (% of total lead)
Greater than 3/8"	18.85	10	0.20
Between 4-mesh and 3/8"	4.53	50	0.24
Between 4- and 10-mesh	3.65	108	0.43
Between 10- and 50-mesh	11.25	165	2.00
Between 50- and 200-mesh	27.80	836	25.06
Less than 200-mesh	33.92	1,970	72.07
Totals	100%	927 (wt-averaged)	100%

Adapted from ITRC (2003)

Is the Subsample Support Representative?

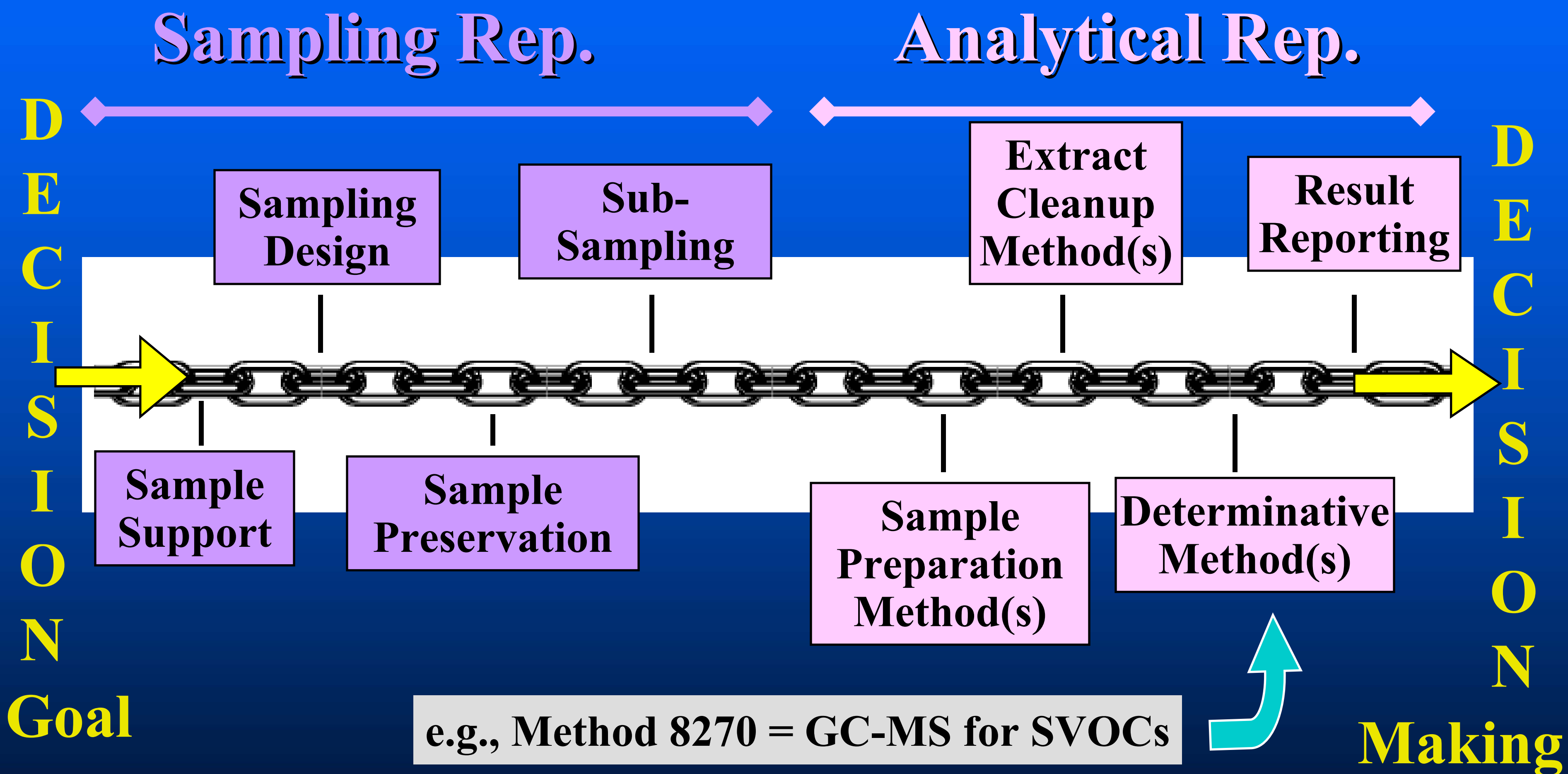
^{241}Am Concentration Varies w/ Subsample Support

Subsample Support (after sample was dried, ball-milled, sieved <10-mesh)	Coefficient of Variation	Number of subsamples required to estimate the sample true mean ± 25% *	Number of subsamples required to estimate the sample true mean ± 10% *
1 g	0.79	39	240
10 g	0.27	5	28
25 g	0.30	6	35
50 g	0.12	1	6
100 g	0.09	1	4

Adapted from DOE (1978)

* Using classical parametric statistics at 95% confidence

The Data Quality "Chain"



All links in the Data Quality chain must be intact for data to be representative of the decision!

Second Generation Data Quality Model

Scientific Foundation

- "Data quality" = assessed per data's ability to support decisions
- Anything that compromises data's ability to represent actual site with respect to the decision compromises data quality
- Environmental matrices must be assumed heterogeneous over small scale distances unless proven otherwise
- "Data" representativeness = sampling representativeness + analytical representativeness
- Project-specific planning: matches scale(s) of data generation (sampling + analytical) with scale(s) of decision-making.
- Technical expertise is required to manage sampling and analytical uncertainties

Summary: New Technologies Provide Significant Benefits

- **Many of the benefits provided by new data generation technologies stem from their ability to provide**
  - A higher density of data points
  - Real-time turnaround of results
- **This combination <u>decreases</u> costs of investigation & cleanup while <u>increasing</u> decision confidence!**
  - Higher resolution data can characterize contaminant heterogeneity at finer scales → More accurate CSMs
    - » Better data representativeness
    - » More accurate decisions about risk
    - » More cost-effective risk management designs
    - » Faster, more effective cleanups

Managing Decision Uncertainty Using Modern Tools and Strategies

Fostering Change

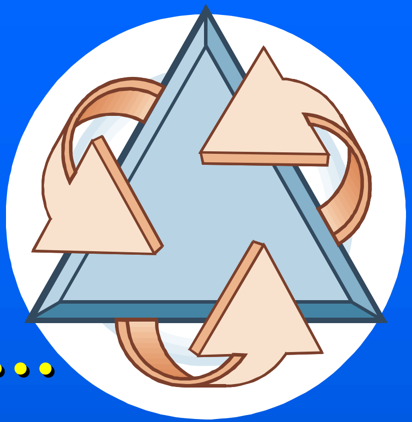
"You never change things by fighting the existing reality. To change something, build a new model that makes the existing model obsolete."

—Buckminster Fuller

A Systems Approach Framework
The Triad Approach

Synthesizes practitioner experience, successes, and lessons-learned into an institutional framework

Unifying Concept for Triad: Managing Uncertainty



Systematic planning is used to proactively…

- **Manage uncertainty about project goals**
  - Identify decision goals with tolerable overall uncertainty
  - Identify major uncertainties (cause decision error)
  - Identify the strategies to manage each major uncertainty
- **Manage uncertainty in data**
  - **Sampling uncertainty:** manage sample representativeness
  - **Analytical uncertainty:** especially if field methods are used
- **Multidisciplinary expertise critical**
  - **A TEAM** is the best way to bring needed knowledge to bear

Allied Environmental Professionals

- Many parallels between the medical and environmental industries
  - Work to maintain & restore health and well-being
  - Medical testing techniques adapted to support cleanup industry (e.g., immunoassays)
- The medical field changed with advancing technology
  - Specialization: Went from "old country doctor" doing everything to a team of "allied health professionals" specifically trained in different diagnostic techniques and treatments
- Is the environmental field ready to modernize?
  - Are we ready to recognize the benefits of specialization to wield advanced technology tools & treatments properly (e.g., geophysicist, chemist, soil scientist, engineer, hydrogeologist, regulatory expert, risk assessor, statistician, sampler, ecologist)

Catalyzing Change

I am personally convinced that one person can be a change catalyst, a transformer in any situation, any organization. Such an individual is yeast that can leaven an entire loaf.

It requires vision, initiative, patience, respect, persistence, courage, and faith to be a transforming leader.

-- Stephen R. Covey

Dynamic Work Plan Strategy

- Real-time decision-making "in the field"
  - Evolve CSM in real-time
  - Implement pre-approved decision tree using senior staff
  - Contingency planning: most seamless activity flow possible to reach project goals in fewest mobilizations
- Real-time decisions need real-time data
  - Use off-site lab w/ short turnaround?
    - » Use screening analytical methods in fixed lab?
  - Use on-site analysis?
    - » Use mobile lab with conventional equipment?
    - » Use portable kits & instruments?

Mix And Match

In all cases, must generate data of <u>known</u> quality

Generating Real-time Data Using Field Methods

Manage Uncertainty through Systematic Planning

- **Need clearly defined data uses—tie to project goals**
- **Understand dynamic work plan—branch points & work flow**
- **Project-specific QA/QC protocols matched to intended data use**
- **Select field analytical technologies to**
  - Support the dynamic work plan (greatest source of $$ savings)
  - Manage sampling uncertainty (improves decision quality)
- **Select fixed lab methods (as needed) to**
  - Manage uncertainties in field data (just ONE aspect of QC for field data)
  - Supply analyte-specific data and/or lower quantitation limits (if needed for regulatory compliance, risk assessment, etc.)

The Strengths & Limitations of Methods

Costly "definitive" analytical methods

↓

Low DL + analyte specificity

↓

Manages analytical uncertainty
= analytical representativeness
= analytical quality

"Definitive" analytical quality
Screening sampling quality

Cheaper (screening?) analytical methods

↓

High spatial density

↓

Manages sampling uncertainty
= sampling representativeness
= sampling quality

Builds CSM

"Definitive" sampling quality
Screening analytical quality

Screening Quality Data

Data Quality for Heterogeneous Matrices

Cheap (screening?) analytical methods → High spatial density → Manages CSM & sampling uncertainty

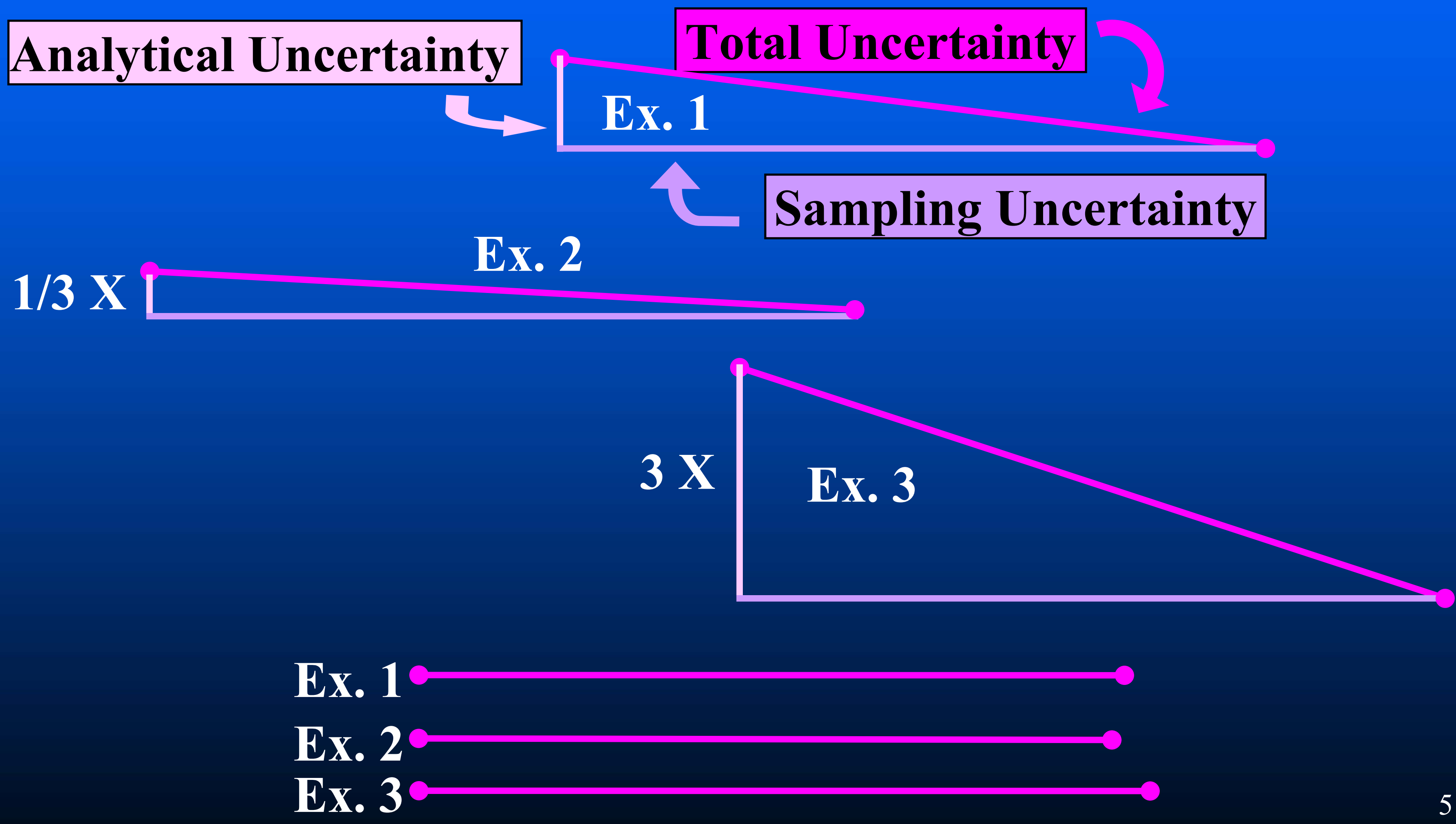
Costly definitive analytical methods → Low DL + analyte specificity → Manages analytical uncertainty

Collaborative Data Sets

Collaborative data sets complement each other so that all sources of data uncertainty important to the decision are managed

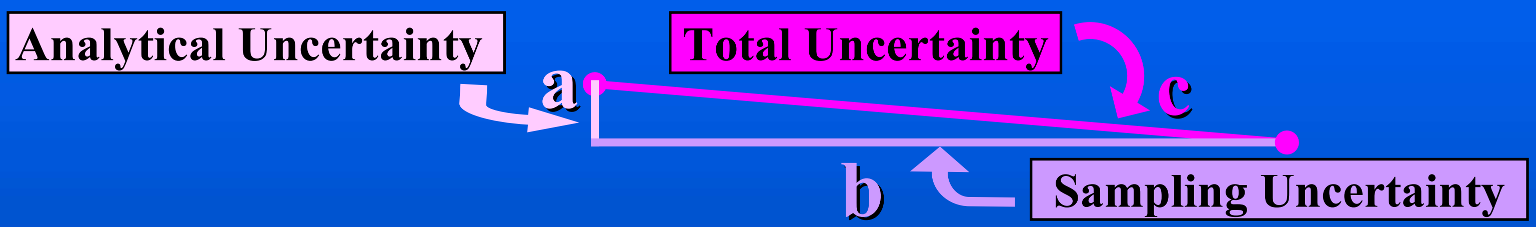
Summing Uncertainties

Uncertainties add according to ($a^2 + b^2 = c^2$)



Partitioning Data Uncertainty

Brownfields Project Example: Scrap yard site w/ contaminated soil



$\text{Std Dev}_{\text{Sampling}} : \text{Std Dev}_{\text{Analytical}}$ = Samp:Anal Ratio

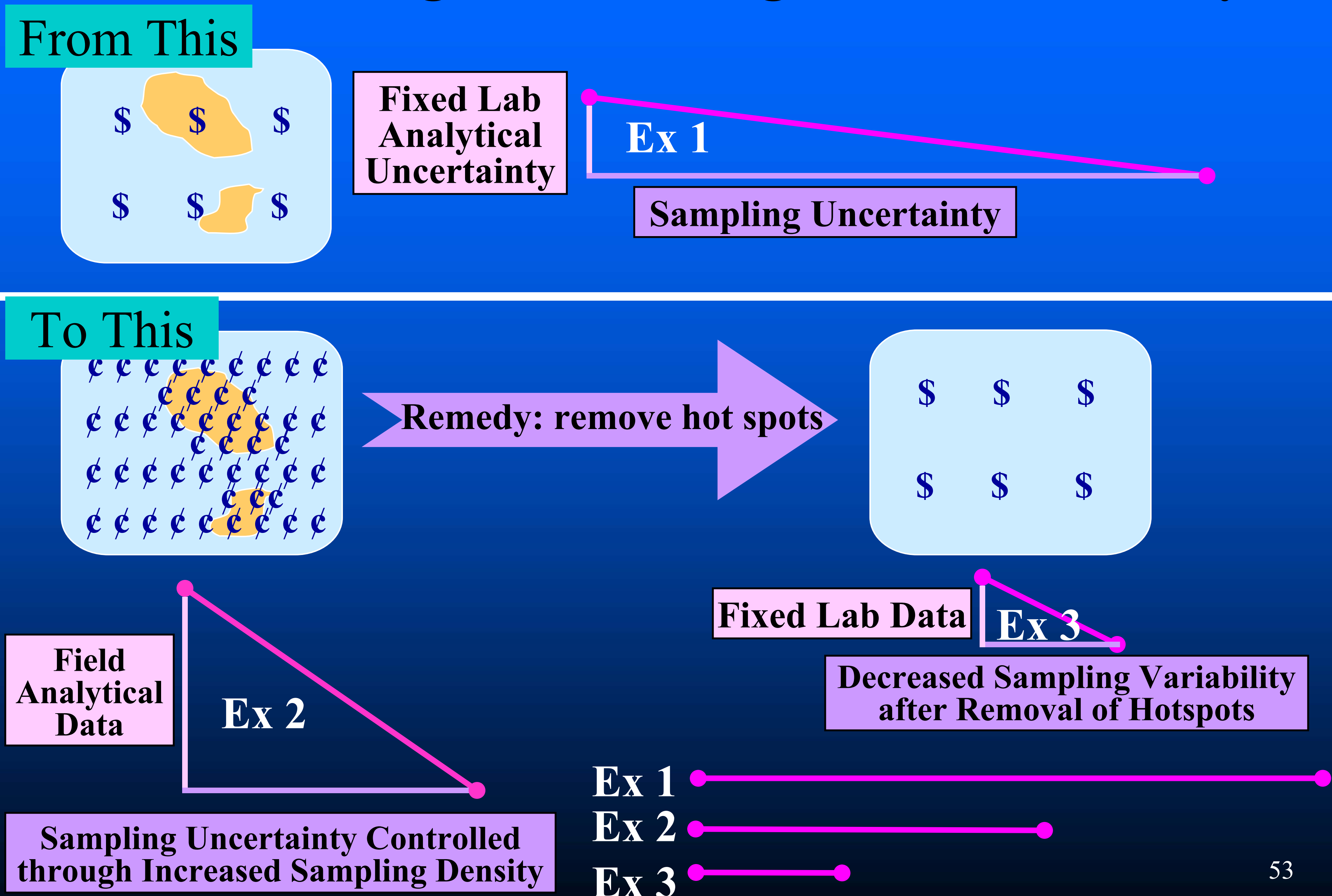
Different metals (LCS data used to estimate analytical variability)

Natural background present, As	22.4 : 7	=	3 : 1
High spatial variability, Pb	3255 : 3	=	1085 : 1

A 3:1 ratio for sampling-to-analytical Std Dev = 90% of statistical variance due to non-method considerations

A 1000:1 ratio for sampling-to-analytical Std Dev = 99.999% of statistical variance due to non-method considerations

A New Paradigm that Manages Decision Quality



Sample Representativeness is Key!

Finally able to address **defensibly and affordably!**

- **Cheaper analyses permit increased sample density**
  - New software for statistical/geostatistical decision support
    - » VSP software pkg FREE: http://dqo.pnl.gov/VSP/index.htm
    - » SADA software pkg FREE: http://www.tiem.utk.edu/~sada/
    - » FIELDS/SADA software: http://www.epa.gov/region5fields/static/pages/index.html
- **Real-time measurements support real-time decision-making**
  - Rapid feedback for course correction → smarter sampling
- **Data Quality: Focus on overall data uncertainty; analytical uncertainty usually a small fraction**

Internally Consistent Terminology to Anchor Data Quality Concepts in Uncertainty Management

Triad Terminology: Quality Assurance

- **Project QA: ID causes of potential decision errors & the strategies to manage them w/ transparent documentation**
- **Data QA: Manage <u>both</u> sampling and analytical uncertainties to degree needed**
  - Analytical representativeness evaluated, including impact of sample/matrix effects on analytical performance
  - Sample representativeness evaluated
- **Lab QA: Manage technical performance of analytical instruments, processes, and operators to meet lab proficiency goals**
  - Sample/matrix effects on analytical performance may or may not be evaluated—depends on contract specifications.

Representativeness for Environmental Contaminant Cleanup

- **Decision Support** = the spatial dimensions & physical properties that define the population about which a particular environmental decision will be made (i.e., the physical dimensions of the decision unit = a population subject to a distinct decision).
- **Sample Support** = the spatial dimensions & physical properties of a sample that is representative of the decision unit.
- Because contamination is heterogeneous, an accurate CSM must depict the separate decision units present on-site. A representative CSM is one that accurately resolves decision unit boundaries at the scale required to make a correct decision.
- "Representative samples" are those that
  - Help define the boundaries of the populations/decision units (i.e., help refine the CSM to achieve a desired level of CSM accuracy) OR
  - Are taken from previously defined populations to determine population characteristics (such as the mean and extremes of a population).

Misleading Terminology

Misleading because…

- Not all methods run in the field are screening methods!
- Not all data produced in the field are screening quality data!
- Fixed labs using definitive analytical methods may produce screening quality data!
- Screening methods can (and should) be used more often in fixed labs to better manage sampling uncertainty and improve analytical performance of traditional methods.

Triad Terminology: Data Quality

- **Collaborative data sets** = distinctly different data sets (i.e., produced by different methods that might not be statistically comparable) used in concert with each other to co-manage sampling and analytical uncertainties to an acceptable level. Usually this is the most cost-effective way to generate decision quality data.
- **Decision quality data* = Effective data* =** data shown to be effective for decision-making (see extended definition, slide 32)
- **Screening quality data* =** some useful information is provided; but too much uncertainty present to support decision-making if used alone. [Note: Applies to both excessive analytical or sampling uncertainties, therefore applies to data produced by definitive analytical methods if the sampling representativeness is uncertain.]

* Includes sampling uncertainty. Nature of the analytical method irrelevant.

"Effective Data"
"Decision Quality Data"

Data of
known quality
that can be logically demonstrated to be
effective for making the specified decision
<u>because</u> both the
sampling and analytical uncertainties
are managed to the degree necessary to meet clearly defined
(and stated) decision confidence goals

Accept NO Imitations!

Project-specific claims for "effective data" are void & meaningless unless decisions and decision supports are specified in plans!!!

On-Line Resources

- EPA TIO Triad information: http://cluin.org/triad
  - ES&T "Managing Uncertainty in Environmental Decisions" article: http://cluin.org/download/char/oct01est.pdf
  - Quality Assurance journal "Representativeness" article: http://cluin.org/download/char/dataquality/dcrumbling.pdf
  - Remediation journal "Next-Generation Practices" article: http://cluin.org/download/char/spring2003v13n2p91.pdf
- EPA TIO general site characterization information: http://cluin.org/char1.cfm
- EPA/USACE on-line site characterization technologies "encyclopedia": http://fate.cluin.org
- ITRC diffusion sampler documents: http://itrcweb.org

The Diffusion of Innovation

"At first people refuse to believe that a strange new thing can be done, then they begin to hope it can be done—then it is done and all the world wonders why it was not done centuries ago."

—Francis Hodges Burnett